Table S3. Number of H-bonds and salt bridges formed between residues of the oxidized RBD and ACE2 proteins. The values are obtained in the same way as mentioned in Table S1.

|  |  |  |  |
| --- | --- | --- | --- |
| region of RBD | oxidized RBD-ACE2 | number of H-bonds | number of salt-bridges |
| II&III | Lys417-Asp30 | 0.38 ± 0.05 | 0.89 ± 0.06 |
| III\* | Gly502-Lys353 | 0.38 ± 0.05 | - |
| Thr500-Asp355 | 0.34 ± 0.08 | - |
| Gln498-Lys353 | 0.18 ± 0.10 | - |
| Gln493-Glu35 | 0.15 ± 0.05 | - |
| Tyr505-Glu37 | 0.13 ± 0.06 | - |
| Gly496-Lys353 | 0.11 ± 0.05 | - |